In/Si(111): Self-assembled two-dimensional electron gas

Eli Rotenberg,[1] H. W. Yeom,[2] J. Schaefer,[3] B. Krenzer,[4] M. Rocha,[4] S. D. Kevan[4]

[1]Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, California 94720
[2]ASSRC & Institute of of Physics and Applied Physics, Yonsei University, 134 Shinchon, Seoul 120-749, Korea
[3]Department of Physics, University of Augsburg, Germany
[4]Department of Physics, University of Oregon, Eugene, Oregon 97403

INTRODUCTION

Owing to the high kinetic energy of free electrons, the metallic state is favored only when the potential energy of the ions dominates this kinetic energy. In this situation, the symmetry of the solid dictates that bands are partially-filled, according to simple, single-particle theory. Many body effects beyond the single electron model can introduce new symmetry breaking factors, which under mean field theory, set in below a critical temperature T_c. Electrons are removed from the Fermi level, leading to a variety of interesting ground states of metals, of which high-T_c superconductivity in layered perovskites is only one example.

Such many-body effects are often enhanced at low dimensionality because with fewer degrees of freedom, the quasiparticles overlap more and hence interact more readily. Low dimensional metals are therefore interesting for probing how many body effects impact electronic structure and it is interesting to search for model low-dimensional systems. The most ideal arrangement would be to grow a single monolayer on a semiconducting or insulating substrate in order to eliminate coupling between metal overlayers and the substrate states.

We report measurements of an In on Si(111) self-assembled structure which behaves electronically as a prototypical two-dimensional electron gas (2DEG). The films are characterized structurally with low energy electron diffraction (LEED) and x-ray photoelectron diffraction (XPD). The electronic structure is characterized with Fermi surface mapping and bandmapping. Angle-resolved photoemission measurements were obtained at BL7.0 of the ALS. Samples were created by evaporating In at room-followed by annealing.

Two $\sqrt{7}x\sqrt{3}$ reconstructions – pseudo hexagonal ("hex") and pseudo rectangular ("rect") were reported by Kraft et al to coexist on the same sample for coverages near one monolayer[1] In order for us to achieve pure, single domain $\sqrt{7}x\sqrt{3}$-rect samples, we overexposed the samples to In, and then annealled away excess In at ~300C. The absence of multiple domains, not previously reported, was encouraged through the use of vicinal Si(111) wafers, which were miscut approximately 2 degrees towards the [1,1,-2] azimuth.

Fig 1a shows the atomic arrangement of the $\sqrt{7}x\sqrt{3}$ reconstruction which was determined by Kraft et al.[1] To a first approximation, the In atoms are arranged in a slightly distorted square lattice similar in dimensions to an isolated In(001) layer. The In atoms within the $\sqrt{7}x\sqrt{3}$ unit cell are not equivalent because of the variety of underlying Si bonding geometries. Neglecting the $\sqrt{7}x\sqrt{3}$ superstructure, we consider the atoms to lie in a "1x1-rect" lattice. This is to be distinguished from the underlying, hexagonal Si 1x1 lattice.

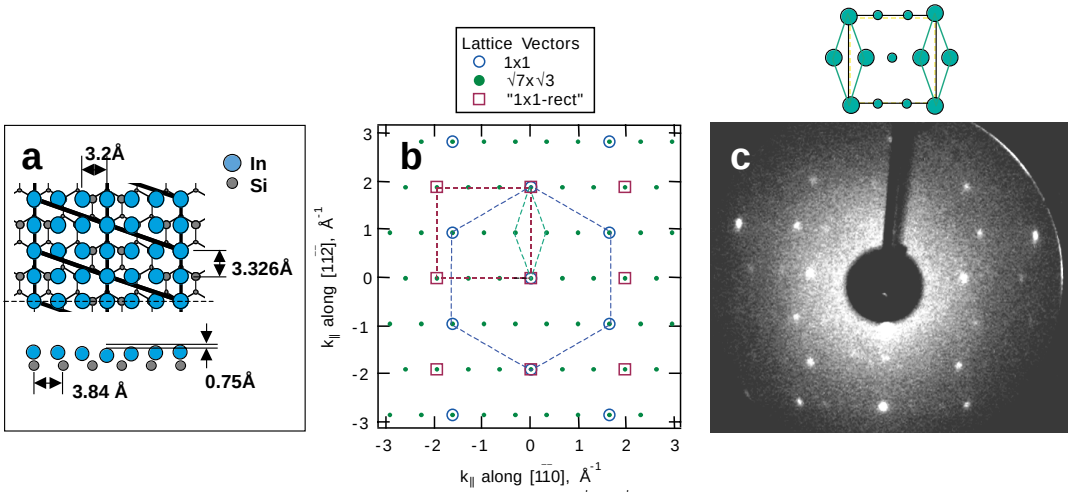

Figure 1. Structural model and diffraction pattern for √7x√3 In/Si(111). (a) Model proposed by Kraft et al (b) positions of principle reciprocal lattice points. (c) LEED pattern obtained. The inset shows the unit building block of this pattern; the spot sizes indicate the relative intensity averaged over energy.

Figure 1b shows the principle LEED diffraction spots to be expected for the three lattices present: 1x1 (i.e. Si), 1x1-rect and √7x√3-rect. The particular atomic basis within the √7x√3 ("hex" or "rect") could modify the spot intensities through a structure factor. In practice, Figure 1c shows the LEED pattern we obtained. We find the pattern to be dominated by the 1x1-rect spots, although all the √7x√3 spots are showing up in the LEED pattern to a greater or lesser extent. The inset to figure 1c shows a cartoon of the basic building block of the LEED pattern, with circles to indicate the relative spot intensity taken over various beam energies. In order to distinguish between the rectangular and hexagonal √7x√3 polytypes, we performed x-ray photoelectron diffraction (XPD) measurements of the In 4d core level (not shown). We found strong evidence for local 4-fold ordering, so we conclude that we achieved a preparation of a pure, single-domain rectangular √7x√3 reconstruction. This is fully consistent with the dramatic Fermi surface measurements reported next.

Figure 2a shows a survey of the momentum distribution of the density of states near E_F. The same data are symmetrized in figure 2b by the known mirror planes, together with the surface Brillouin zone boundaries (BZBs) which are present in the system. We took this data over a larger azimuthal range but with coarser sampling (not shown) in order to verify the correctness of our symmetrization. The most dramatic feature is a more or less square array of very sharp circular contours, which can be simply understood in terms of a trivalent metal on a slightly distorted square lattice (figure 2c). A parabolic nearly free electron band emanates from each Γ point of the reciprocal 1x1-rect lattice. Sampling a constant energy contour at E_F reveals circular cross sections of these parabaloids. Additional features, which we originally supposed to be caused by the presence of weaker minority domains rotated 120-degrees, can in fact be understood by locating additional parabolic bands centered on the subsidiary √7x√3 spots found in the LEED pattern, which act as additional Γ points. We only needed to consider the principle LEED spots to account for nearly all of the remaining features (figure 3d). Due consideration must be placed on the strong matrix element effects, which cause the intensity over most of the subsidiary Fermi contours to be negligible away from the region near the strongest LEED spots.

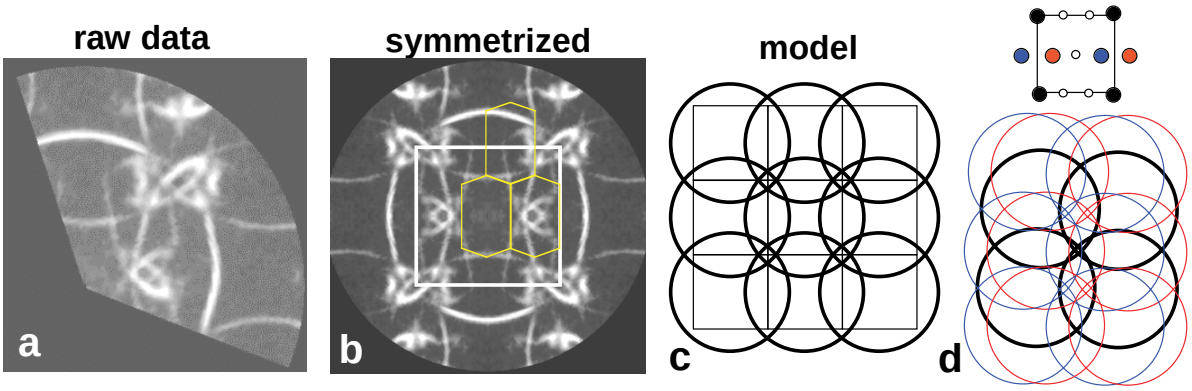

Figure 2. Fermi surface results for √7x√3 In/Si(111). (a) raw data (b) symmetrized by rotation and mirror planes. (c) Simple model assuming 1x1-rect arrangement of In atoms. (d) model including additional free electron bands centered on √7x√3 Γ points.

It is noted in Figure 2b that the √7x√3 BZ boundary happens to align exactly with the Fermi contours along the [1,1,-2] direction (upwards in figure). This coincidence suggests that the unusual reconstruction may be partially stabilized by electron energy gap formation as the bands cross the zone boundary. In fact we find via bandmapping that backfolded bands from the √7x√3 symmetry are clearly visible for the bands in this direction.

To summarize, we have found that a pure, single-domain two-dimensional metallic In layer can be prepared on Si(111) substrates. This material has signatures of a nearly ideal two-dimensional electron gas, with local pseudo-4-fold symmetry, and its electronic structure is dominated by the potential energy distribution of a slightly distorted square ("1x1-rect") lattice. Nevertheless, the external potential of the substrate atoms has some.effect on the electronic structure and indeed the interplay between the periodicities (1x1-rect and √7x√3) may contribute to the stability of the system.

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Principal investigator: Eli Rotenberg, Lawrence Berkeley Laboratory, Erotenberg@lbl.gov, 510-486-5975

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